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EFFECTS OF VACANCIES NEAR SUBSTITUTIONAL IMPLANTS ON TRAPPING AND DESORPTION OF HELIUM – A SIMULATION

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Trapping of He by vacancies and drainage of He from substitutional implants (Ag and Kr in W) to nearby vacancies are investigated using static lattice calculations. The calculations indicate that drainage of He will occur to vacancies within a radius of 2.5 lattice units from the implant. Furthermore the trapping probability of substitutional and interstitial random walkers on a bcc lattice by substitutional traps or vacancies is calculated. When implantation-produced vacancies are present in the vicinity of the observed trap a shielding effect occurs. Trapping constants are calculated with two random walk models for both the unshielded and the shielded defect. For the latter several configurations were taken. The results show that shielding of a defect by one vacancy at a distance of three lattice units leads already to a reduction of He trapping by that defect of 30% to 40%.

1. Introduction

In radiation-damage experiments particles are often used as probes for defects, e.g. He atoms in thermal helium desorption spectrometry (THDS). In THDS He is injected with low energy. After initial penetration of the surface to a depth of several tens of ångströms the He atoms thermalize and start a random walk, see refs. [1,2]. A small fraction of the He atoms is trapped by defects present, the majority escapes at the surface.

For specific defects in the presence of other defects shielding effects will occur, leading to a reduced trapping probability of the random walker by these defects. Especially in the case of damage introduction by ion implantation defects are not distributed homogeneously despite the low doses often applied: defects made in a single collision cascade are often close to each other. A recent study in which perturbed angular correlation measurements (PAC) were compared with THDS to investigate defects in W after 25 keV Ag implantation at low doses ($< 10^{13}$ Ag⁺ cm⁻²) demonstrates this [3]. PAC reveals a near 100% substitutional fraction of Ag after implantation, whereas with THDS substitutional implants can only be detected after annealing to 1400 K. Since with PAC the decay of an active Ag atom is observed, this method will only probe the Ag atom and

its immediate surroundings. The discrepancy can be explained assuming the presence of nearby vacancies at Ag which either shield Ag for the migrating He atom or which may cause drainage of He trapped at Ag to nearby vacancies or which retrap dissociated He. In a preceding study it was shown with binary collision cascade simulations that indeed an average of one to three nearby vacancies may be expected within a distance of four lattice units from the implanted atom [4]. During annealing a large fraction (40–60%) of these vacancies will migrate to the implant, as observed with PAC.

In sect. 2 attention is given to the possibility of He drainage from implanted atoms to nearby vacancies and retrapping of He in nearby vacancies during the desorption step in THDS.

In sect. 3 the situation prior to annealing is taken to calculate the shielding effects of nearby vacancies on He trapping by implanted atoms (sect. 3). Different vacancy–implant separations and configurations were taken and studied with random walk simulations.

2. He drainage from implants to nearby V

2.1. Static lattice calculations

Static lattice calculations were used to calculate trapping positions, dissociation paths and dissociation energies of He at a vacancy, at a substitutional Kr atom and at a substitutional Ag atom in W. The defects were placed in the centre of a small crystallite ($17 \times 17 \times 17a_0^3$ with a_0 the lattice constant). The W–W potential de-

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scribing the pair interaction of the tungsten atoms was fitted to elastic constants by Johnson and Wilson [5]. The He-Kr, He-W and Kr-W potentials were calculated by Baskes [6] using the modified Wedepohl method [7,8]. The Ag-W potential was obtained by scaling of the W-W potential [9]. The He-Ag potential was constructed using the modified Wedepohl method [8,9]. Dissociation and migration energies were obtained by calculating the total energy of the crystallite with the dissociating or migrating particle held fixed at various positions along the dissociation respectively migration path. The crystallite was allowed to relax fully.

2.2. Trapping of He at V and KrV/AgV

According to calculations of ref. [5] He in W migrates from octahedral across tetrahedral to octahedral position with a migration energy of 0.25 eV (the octahedral position is the midpoint of the edge of the bcc cell, the tetrahedral position is the midpoint between two neighbouring octahedral positions). This allows the He atom to jump in four directions with jumping distance $a_0/2$. The nearest lattice and octahedral positions at a trap are shown and labelled in figs. 1a and 1b and table 1. Units of $a_0/2$ are used further in the text. For a vacancy as trap and He as migrating particle the octahedral site 2 is a trapping position. For site 3 being a trapping position either migration of He to site 2 or migration of the lattice atom at (2, 0, 0) to the vacancy at (0, 0, 0) with He simultaneously jumping into the newly created vacancy is required. The first process is calculated to have the same tetrahedral saddlepoint energy as for bulk migration of He. The latter reaction, He assisted vacancy jumping, has been investigated by Wilson and Bisson [10]. They found that it requires the same energy as bulk vacancy migration. Thus site 3 can be excluded as He trapping position. For He positioned at site 4 and site 5a calculations were also performed of the energy required to move the atom at (1, 1, 1) into the vacancy. The energies relative to the energy of the crystallite with He trapped in a vacancy (V) are shown in fig. 2. It should be noted that ref. [10] had already calculated this for the first position, but for He fixed at positions along the line connecting (0, 0, 0) and (1, 1, 1), He and the surrounding lattice atoms were allowed to relax fully.

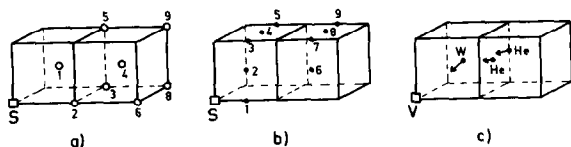


Fig. 1. The nearest lattice positions (a) and octahedral positions (b) at a sink *S* and a schematic representation of He assisted vacancy jumping (c).

Table 1

Coordinates in $a_0/2$ of the n th nearest neighbour position with respect to site (0, 0, 0) for lattice positions (V's) and octahedral positions (He) in a bcc lattice

<i>n</i>	V	He
1	(1, 1, 1)	(1, 0, 0)
2	(2, 0, 0)	(1, 1, 0)
3	(2, 2, 0)	(2, 1, 0)
4	(3, 1, 1)	(2, 1, 1)
5	(2, 2, 2)	a (2, 2, 1) b (3, 0, 0)
6	(4, 0, 0)	(3, 1, 0)
7	(3, 3, 1)	(3, 2, 0)
8	(4, 2, 0)	(3, 2, 0)
9	(4, 2, 2)	a (3, 2, 2) b (4, 1, 0)
10	a (3, 3, 3) b (5, 1, 1)	a (3, 3, 0) b (4, 1, 1)

The results indicate that He at positions 4 and 5a will push the tungsten atom into the vacancy, thereby itself being trapped by the newly formed vacancy. The reaction is visualized in fig. 1c.

In fig. 3 energy variations are shown of the crystallite if a He atom is moved along the path connecting the position of He trapped at substitutional Ag or Kr and the octahedral site 6 of fig. 1b. From the figure it clearly follows that site 3 (in the figure He at a_0) is a trapping position for He.

2.3. Drainage of He from KrV/AgV to and retrapping in nearby V/HeV

Drainage either at room temperature or during desorption takes place when the energy required for He to reach a nearby V or nearby HeV is below the normal dissociation energy.

Instead of calculating all possible drainage paths in the vicinity of a V we followed a simplified approach.

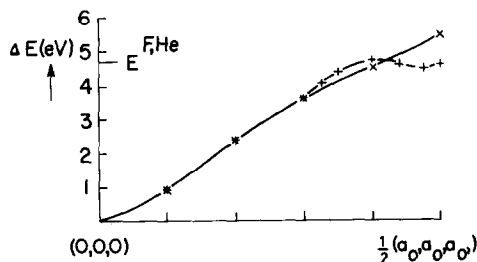


Fig. 2. Migration energy of a W atom along the $\langle 111 \rangle$ direction near a vacancy at (0, 0, 0) in the presence of a He atom, initially at site 4 (x), or at site 5a (+). Both He and the surrounding W atoms were allowed to relax fully.

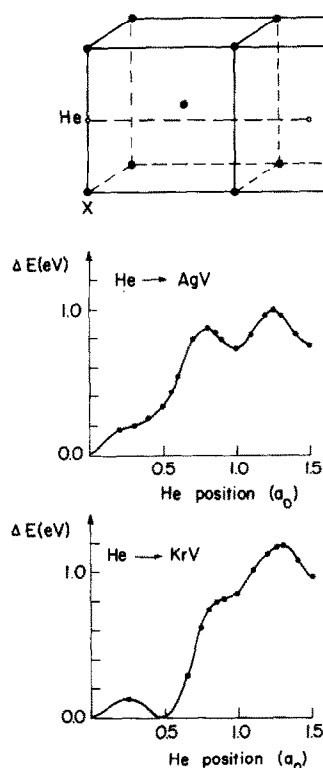


Fig. 3. Energy variation of a W crystallite with He fixed at various positions along the [100] axis close to substitutional Ag and Kr.

We assumed that the energy variation as calculated in sect. 2.2 (fig. 3) for He dissociating from KrV or AgV will not be altered by a nearby V. Then the problem of finding the drainage paths is reduced to determining all trapping positions for He at an n th neighbour V which can be reached by He originally trapped at KrV/AgV with an energy lower than the bulk dissociation energy. For instance a V at a 4th neighbour position (table 1) relative to a KrV will migrate spontaneously to a 2nd neighbour position if a He atom is trapped at a KrV and therefore may be at (1, 1, 0). For a few drainage reactions (5th and 7th neighbour V) the energy variation along the He migration path was followed. For Ag the rule held well, for Kr the rule slightly overestimated the required energies (~ 0.05 eV). In table 2 all drainage reactions which will occur are shown. Energies required for the reactions are also shown. It is clearly demonstrated that drainage is quite effective, especially for He from KrV to a nearby V. For AgV drainage of He under influence of an 8th or 9th neighbour V is only slightly favoured above normal dissociation. It should be realized that if more strain is present, as may be expected when a larger impurity atom is involved or when more than one He atoms are trapped, drainage of He under

Table 2

Energies required for He drainage reactions. Figures between brackets indicate n th neighbour lattice positions.

Reaction	Energy (eV)
HeKrV \rightarrow KrV + He ^{a)}	1.16
HeKrV · V(n) \rightarrow KrV · HeV(n) $n = 1, 2$	0
HeKrV · V(n) \rightarrow KrV · HeV(1) $n = 3, 5$	0
HeKrV · V(4) \rightarrow KrV · HeV(2)	0
HeKrV · V(7) \rightarrow KrV · HeV(3)	0.13
HeKrV · V(n) \rightarrow KrV · HeV(4) $n = 8, 9$	0.85
HeAgV \rightarrow AgV + He ^{a)}	1.00
HeAgV · V(n) \rightarrow AgV · HeV(n) $n = 1, 2$	0
HeAgV · V(n) \rightarrow AgV · HeV(1) $n = 3, 5$	0
HeAgV · V(4) \rightarrow AgV · HeV(2)	0
HeAgV · V(7) \rightarrow AgV · HeV(3)	0.35
HeAgV · V(n) \rightarrow AgV · HeV(4) $n = 8, 9$	0.90
HeKrV · HeV(n) \rightarrow KrV · He ₂ V(n) $n = 1, 2, 3$	0
HeKrV · HeV(4) \rightarrow KrV · He ₂ V(4)	0.83
HeAgV · HeV(n) \rightarrow AgV · He ₂ V(n) $n = 1, 2$	0
HeAgV · HeV(3) \rightarrow AgV · He ₂ V(3)	0.14
HeAgV · HeV(4) \rightarrow AgV · He ₂ V(4)	0.76
HeAgV · HeV(5) \rightarrow AgV · He ₂ V(5)	0.95

^{a)} Dissociation reaction.

influence of an 8th or 9th neighbour V will be more favoured.

Drainage of He to a nearby HeV is less effective because the phenomenon as pictured here that He pushes a W atom in the nearby vacancy will not occur. We assume that the trapping positions relative to the HeV are thus limited to the octahedral sites 2. Calculations of He migration paths were performed. The results indicate that beside the first, second and third neighbour HeV drainage also takes place to a fourth neighbour HeV. For the fifth neighbour HeV only very slight enhanced drainage was found in the case of AgV (see table 2).

In the case of a nearby V to which drainage does not take place still a rather high probability exists of spontaneous retrapping of He after dissociation from an XV ($X = \text{Ag, Kr}$). In [11] it is shown that the probability of trapping in a near sink with sink radius r_s at distance R versus escape at infinity is given by r_s/R . In desorption experiments the surface is nearby, thus the fraction being retrapped after dissociation will be lower. To obtain an estimate of this effect a simple random walk model was applied. A random walker started a 1000 times at octahedral positions around the origin in a box of $16 \times 16 \times 16 a_0^3$ containing a vacancy at a certain distance from the origin. Capture criteria for He close to a V followed from section 2.2, the random walker was assumed to escape if at the edge of the box. The trapping probabilities calculated this way, combined

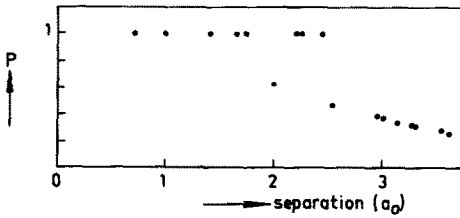


Fig. 4. Probability P for He, initially trapped at XV ($X = \text{Ag, Kr}$), to be trapped in a V , either spontaneously or during annealing, as a function of XV - V separation.

with the drainage probabilities, for different XV - V separations, are used to obtain the fraction of He atoms trapped in a V after initially being trapped in an XV . The result is shown in fig. 4.

3. Random walk simulations

3.1. Periodically arranged traps

In the preceding study [4] concerning vacancy trapping by substitutional noble gas atoms a random walk model was used which could be related with diffusion theory to obtain effective trapping constants for defects. Hitherto the average lifetime $t_{av,rw}$ of a random walker in a periodic array of spherical sinks with concentration c_s was calculated. $t_{av,rw}$ thus calculated was compared with the average lifetime $t_{av,d}$ of a particle diffusing in a sphere with boundary conditions $dc/dt = 0$ for $x = R$, with R the radius of the sphere, and $c = 0$ for $x \leq r$, so that r is the trapping radius of the defect. The solution of this problem is given by Ham [12]. Fastenau et al. [13,14] compared the diffusion theory with random walk results for different random walker-defect combinations. Interaction of vacancies, self interstitials and He atoms with vacancies were simulated by them. In this study we are mainly interested in He interaction with defects. To simulate the shielding of implanted atoms by vacancies we introduced an extended sink, composed of different traps, in the centre of a crystallite. He atoms leaving the box are entering it at the opposite side of the box, so that the box is equivalent with periodically arranged traps, see also refs. [13,15]. For sinks three different trapping radii were taken, in accordance with the calculations in sect. 2.2. For empty vacancies a rather large trapping volume was taken (see table 3). For a vacancy filled with a small impurity, here HeV, only the site (1, 1, 0) was taken, whereas for larger impurities also the site at (2, 1, 0) was taken as trapping position. The average number of jumps n_{av} for a He atom to be trapped, starting at a random position within the crystallite, was calculated. From diffusion theory the relation between n_{av} and the trapping con-

Table 3

Trapping sites in $a_0/2$ coordinates and calculated trapping constants for interaction of He with various defects

Defect	Trapping sites	Z_0
V	(1, 1, 0) (2, 1, 1) (2, 2, 1)	1.41
HeV	(1, 1, 0)	0.73
XV , $X = \text{Ag, Kr}$	(2, 1, 0)	1.15
$V_2(1)$, $V_2(2)$	as for V	1.67
$V_3(112)$	as for V	1.72
$V_4(111122)$	as for V	1.87

stant Z_{eff} is obtained as follows:

$$dc_m/dt = Z_{eff} \nu c_s c_m, \quad (1a)$$

where ν is the jumping frequency, c_m the concentration of random walkers, c_s the sink concentration and Z_{eff} the trapping constant. Calculation of the average lifetime t_{av} and taking $n_{av} = t_{av} \nu$ it follows:

$$Z_{eff} = \frac{1}{t_{av} \nu c_s} = \frac{1}{n_{av} c_s}. \quad (1b)$$

The trapping constant Z_0 for infinitely low sink concentration c_s and octahedral random walkers on a bcc lattice was calculated by refs. [12–14] to depend on Z_{eff} according to the following relation:

$$Z_0 = \pi (R\alpha - \arctg R\alpha) / 3\alpha, \quad (2a)$$

with R the radius in a_0 of the sphere corresponding with $1/c_s$ atoms, α is given by:

$$\alpha = (9Z_{eff}/\pi R^3)^{0.5}. \quad (2b)$$

An access factor $A_{i,j}$ for a sink U_i near another sink U_j with a total sink concentration approaching zero can be defined:

$$A_{i,j} = f_i Z_{oi,j} / Z_{oi}, \quad (3a)$$

with $Z_{oi,j}$ the trapping constant for the extended sink composed of defects U_i and U_j and f_i the fraction of random walkers trapped in defect U_i . An alternative definition is:

$$A_{i,j} = f_i Z_{eff,i,j} / Z_{eff,i}. \quad (3b)$$

$Z_{eff,i}$ represents the trapping constant for defect U_i at a sink concentration which corresponds with the sink

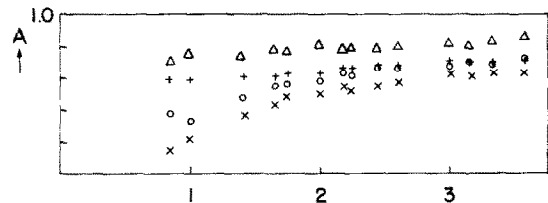


Fig. 5. Access factors of V near V (+), HeV near V (x), XV near V (o) and XV near HeV (Δ) for octahedral random walkers on a bcc lattice as a function of separation.

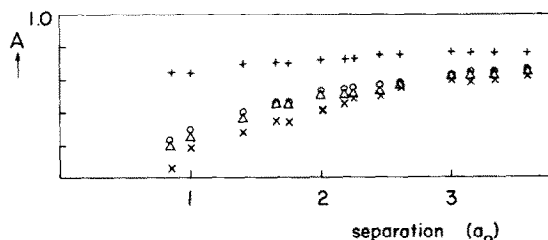


Fig. 6. Access factors of V near V₂ (+), XV near V₂(1) or V₂(2) (O), XV near V₃(112) (Δ) and HeV near V₂ (x), further as in fig. 4.

concentration in the case of defect U_j near U_i , with U_i and U_j counted as separate sinks. The definition has only physical meaning for equal sinks U_i and U_j .

The average number of jumps required for trapping n_{av} was calculated for a sink in the centre of a box of $12 \times 12 \times 12$ a_0^3 . The octahedral random walker was released 3000 times at random positions within the box, trapping positions excluded, for every defect configuration. Thus obtained n_{av} s were substituted in eqs. (1), (2) and (3) to calculate access factors for V near V, HeV near V, XV near V and XV near HeV (see fig. 5). For those trapping sites around a HeV or XV at which He can be trapped by the V as well preference was given to trapping by the V. The trapping constants at infinitely low concentration and the trapping sites are given in table 3. The access factor is typically between 0.4 and 0.6 depending on the combination and separation. For two HeV's also a calculation was performed for a larger separation. The value of A approaches 1 as may be expected. In fig. 6 the access factors of V's and XV's near a di- and tri-vacancy are shown. Again for octahedral sites within trapping distance of both defects the di- or trivacancy was supposed to be the stronger trap. The distance between the nearest vacancy of the di- or tri-vacancy and the sink is taken as separation. The di-vacancy was taken either as V₂(1) or V₂(2); a nearest neighbour V₂ or a second nearest neighbour V₂. For the tri-vacancy the most stable one was taken; V₃(112) according to refs. [16,17]. In fig. 7 the fraction He trapped by XV in the presence of V, V₂ and V₃ is shown.

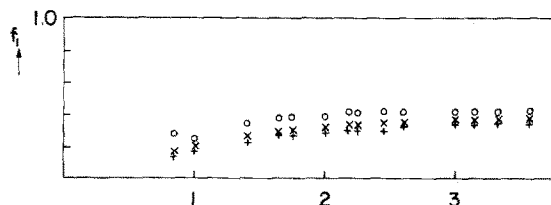


Fig. 7. Fraction of octahedral random walkers trapped by XV in the presence of V (O), V₂ (x) and V₃ (+) as a function of separation.

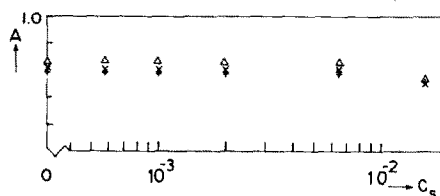


Fig. 8. Access factor for V near V as a function of the sink concentration, (+) first neighbour separation, (x) third neighbour and (Δ) ninth neighbour separation.

To investigate the dependence of the access factors on the total sink concentration for a first to tenth neighbour divancy calculations of the (imaginary) mutual shielding were performed for different sink concentrations using eq. (3b). In fig. 8 a few illustrative results are shown. Access factors at infinitely low concentration are also shown. It should be noted that the coincidence of the access factors at concentration zero with the factors at 5.8×10^{-4} reflects the fact that Z_0 was calculated from n_{av} at this concentration. The figure demonstrates that eq. (3b), if applicable, is equivalent with eq. (3a). Deviations occur if the size of the extended sink is not small compared with the size of the crystallite.

The periodicity of the sinks in general leads to a higher Z_{eff} than for randomly distributed sinks with a similar concentration. In ref. [18] Z_{eff} for He trapping by vacancies for both cases was calculated. For sink concentrations below 10^{-3} the two values approach each other. So we expect that the shielding factors found above for the periodic arrangement differ little from shielding factors for random sink arrangements at vacancy concentrations below 10^{-3} .

3.2. Shielding at infinitely low defect concentration

To calculate the effective shielding directly at infinitely low defect concentration another approach can be used. Consider the trapping positions around defect and neighbouring vacancies again as an extended sink. It was shown by Soos and Powell [19] that the random walk of a point defect in a crystal containing m extended defects is equivalent with the random walk of an extended sink (including all trapping positions) in a crystal containing m immobile point defects. Fastenau et al. [14,20] used this concept, but now only the number of "fresh" sites $S_n(U_j)$ the extended sink U_j had encountered after n steps was investigated. Montroll and Weiss [21] already showed that for low point defect concentrations $S_n(U_j)$ can be approximated by

$$S_n(U_j) = b(U_j) \cdot n + c(U_j) \cdot \sqrt{n} + d(U_j). \quad (4)$$

$b(U_j)$, $c(U_j)$ and $d(U_j)$ are coefficients of the series

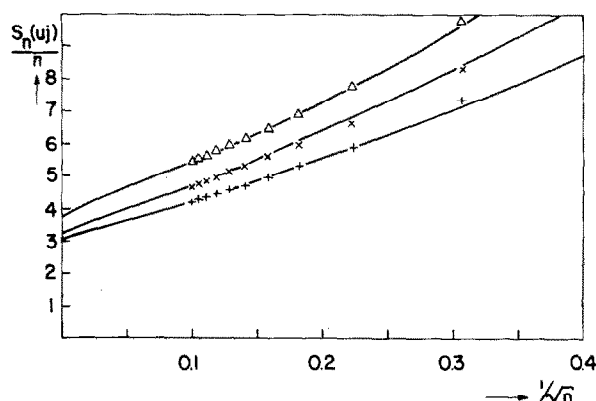


Fig. 9. $S_n(U_j)/n$ vs $1/\sqrt{n}$ for n th neighbour di-vacancies, (+) $n=1$, (\times) $n=3$ and (Δ) $n=9$, marked points are obtained with Monte Carlo simulations, drawn curves are best fits using eq. (4).

expansion of S_n [14]. The physical meaning of relation (4) is that $b(U_j)$ equals Z_0 (see refs. [14,20]). It may be assumed that eq. (4) is also valid for extended defects in three dimensions.

To calculate effective shielding factors for different defect configurations the number of fresh sites encountered by the composite defect as obtained with random walk was fitted with eq. (4). By distinguishing the number of fresh sites encountered by the shielded and the shielding defects and applying eq. (3a) on the $Z_{0,j}$ found the access factor A is obtained.

Since He migrates interstitially random walkers on an imaginary lattice should be concerned. Koiwa and Ishioka [22–24] have treated this problem in a series of articles for point defects. Their theoretically obtained results agree with the random walk calculations of Fastenau (Koiwa: $b = 0.5713$, Fastenau: $b = 0.567$). For

Table 4

Parameters describing the random walk of an extended sink on a bcc lattice as obtained with eq. (4) from Monte Carlo simulations and access factors A . Defects were allowed to jump in the $\langle 111 \rangle$ direction. All first neighbour positions were taken as trapping positions.

Defect	$b(U_j)$	$c(U_j)$	$d(U_j)$	A
V	2.42	7.97	2.02	–
$V_2(1)$	3.06	10.44	9.35	0.63
$V_2(2)$	3.17	10.38	7.91	0.65
$V_2(3)$	3.23	13.75	10.16	0.67
$V_2(4)$	3.45	14.17	7.30	0.71
$V_2(5)$	3.50	13.51	10.16	0.72
$V_2(6)$	3.73	13.46	13.19	0.77
$V_2(7)$	3.78	13.64	13.75	0.78
$V_2(8)$	3.66	16.53	5.77	0.76
$V_2(9)$	3.83	14.77	13.24	0.79

Table 5

Access factors of XV near several vacancies for octahedral random walkers on a bcc lattice, $X = \text{Ag, Kr}$. The positions of the V's relative to XV are schematically indicated.

Relative positions of V (\square) and XV (\bullet)	A
	0.24
	0.34
	0.42
	0.48

extended defects however the concept of an octahedral walking sink instead of octahedral walking point defect cannot be applied in a straightforward manner. All octahedral trapping positions around the extended sink should perform an octahedral random walk. Thereby they necessarily cross lattice positions which never could have been visited by He atoms. Although this problem can be solved, it requires considerably more calculation time, especially if the more realistic larger trapping radius is taken, and thus we limited ourselves here to random walkers on lattice positions. The random walker was supposed to be trapped once it arrived at a first neighbour position of the trap. Jumps were made to first neighbour positions. Physically this coincides with vacancy migration. For some defects the data thus obtained are shown in fig. 9. Best fits using relation (4) are drawn. $b(U_j)$ is typically about 2–3 times larger than for an octahedral random walker reflecting that the latter can only sample two new lattice positions, whereas the random walker taken here can sample 7 new lattice positions per step. The data thus obtained for $b(U_j)$, $c(U_j)$, $d(U_j)$ and the access factor A are shown in table 4. It can be seen that the access factors are quite similar to the ones calculated in section 3.1.

3.3. Shielding of defects by more than one V

Using the model presented in section 3.1 the effect of different near vacancy configurations was calculated. Crystallite size is taken the same, as well as trapping sites for the octahedral random walker. In table 5 the access factors are shown together with the corresponding defect configurations. For two V's diametrically positioned relative to XV the shielding effect is nearly twice as large as for a single V. For two nondiametrical V's the shielding effect is less than twice as large.

4. Discussion

In general the pair-potential results presented in section 2 will give only a qualitative insight in the processes occurring. the calculated vacancy migration energy of 1.46 eV and the calculated dissociation energy for He from KrV of 1.16 eV are lower than the experimental values (1.8 and 1.7 eV respectively, as derived from the spectra in ref. [25]). We do believe however that the phenomenon of He-assisted vacancy jumping takes place, experimental evidence for this phenomenon is that the reverse reaction (He dissociation) probably takes place in a similar way. Dissociation of He from a singly filled V in W and Mo can only be described by substitution of a pre-exponential factor in the Arrhenius formula for first order desorption which is a factor 100 larger than for vacancies filled with 3 or more He atoms [26,27]. Armstrong et al. [26] proposed that this reflects the higher entropy factor for a process in which a surrounding lattice atom jumps into the vacancy and pushes He out, rather than jumping of He alone. Trapping positions for He around KrV and AgV were also calculated.

The random walk results presented in section 3 are quantitatively reliable. The only uncertainties come from the presumptions concerning the trapping positions. This affects the magnitude of the shielding effect, as can be seen for the various defects with different trapping radii.

Since heating is essential in the experimental scheme of THDS all (thermally activated) drainage reactions requiring a lower energy than bulk dissociation will lead to He desorbing from a V in the experiment. Thus according to the pair-potential calculations only those substitutional implants will be detected with THDS which have either no vacancies within $2.5a_0$ or only at the sixth neighbour position. Furthermore it should be realized that there are only 6 of those out of the 128 n th neighbour positions with $n \leq 9$. Together with the shielding of the sixth neighbour and the retrapping probability of about 0.6 this means that only about 1% of the substitutional implants with a vacancy within $2.5a_0$ will be detected. Various detection probabilities are schematically shown in fig. 10. The results presented in [4] indeed indicate that on the average one vacancy will be present within this distance already at implantation energies of 5 keV for the heavier noble gases in tungsten. So we may assume that the discrepancies between THDS on the one hand, where after implantation only some 5% to 10% of the implants is seen in a substitutional position, and PAC [3] and Mössbauer [28,29] results on the other hand where substitutional fractions between 50% and 90% are seen after implantation, are largely due to combined He drainage and He-assisted vacancy jumping. Retrapping and shielding effects play an additional role.

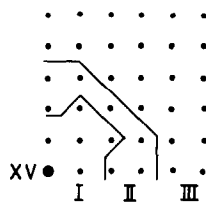


Fig. 10. Detectability of XV in the presence of V with THDS; presence of a V in zone 1 prevents detection; in zone 2, less than 50% will be detected; in zone 3, more than 50% will be detected.

The results presented here also indicate that if THDS is used to deduce total amounts of vacancies produced during heavy ion bombardment, it will tend to underestimate the total number of vacancies produced. The order of magnitude of underestimation will depend on the local vacancy density in the cascade. Especially if vacancy-clustering occurs, the underestimate will be quite drastic. It should be noted that the shielding depends on the He filling degree, a vacancy already filled with a He atom is much less effective in shielding.

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